California Regional PM$_{10}$ and PM$_{2.5}$ Air Quality Study (CRPAQS)

Statement of Work – CRPAQS Data Analysis Task 2.4
ASSESSING BOUNDARY CONDITIONS

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Sonoma Technology, Inc.

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Introduction

Potential control strategies to mitigate particulate matter (PM) concentrations are usually evaluated using an air quality model. These models require that pollutant concentrations and meteorology at the upwind boundary of the modeling region (boundary conditions) be specified. One of the CRPAQS field study objectives is to evaluate and improve the performance of air quality simulations. One aspect targeted for improvement is a better understanding of boundary conditions.

The questions to be addressed in Task 2.4 are as follows:

- What are PM and precursor concentrations at boundary and background sites?

- How do the concentrations vary temporally and spatially?

- How much might these concentrations be biased by local sources?

- What are reasonable values for boundary and background atmospheric compositions to be used for both grid and source apportionment modeling?

- How important are these boundary and background levels when PM$_{2.5}$ and PM$_{10}$ are high at other locations? What is the portion of the total attributable to background? How much of the variance in the high concentrations is attributable to background concentrations?

Much of the current knowledge of boundary and background PM and precursor concentrations in the San Joaquin Valley (SJV) is documented by Collins (1998) based on work performed during the IMS-95, by Watson et al. (1998) in the CRPAQS field plan, and in other related documents (e.g., Magliano et al., 1999). The IMS-95 laid the groundwork for establishing a more detailed network of sites in CRPAQS to provide data to address the objectives of this task. The following three conclusions put forth by Collins (1998) are of note:

1. Clean air and non-anthropogenic background sites did not exist as part of the current network or of previous special study networks (including IMS-95). *All sites showed periods with significant impact from nearby emissions sources.*

The implications for the CRPAQS field study plan resulted in adding sites to better characterize the background and boundary concentrations and composition. Boundary sites added for CRPAQS included Bodega Bay, Sierra Nevada Foothills, and Angiola.

2. Clean air background and sources outside the region do not appear to play a significant role in determining SJV concentrations during fall and winter PM episodes.

More data are now available from the CRPAQS field study to further investigate this finding.

3. Clean air/background site characteristics, transition distances from sub-regional to regional background concentrations are not well-known. Winter stagnation complicates identification of boundary or flux-plane sites—in these cases, conditions at the onset of episode are important to understand (and are the boundary conditions).

We anticipate at least three meteorological regimes under which model simulations will be performed: (1) summer transport conditions, (2) fall/winter transport conditions, and (3) winter stagnation conditions. The boundary conditions including potential boundary sites, pollutant concentrations, and PM composition, will likely be quite different for each episode type given the differences in meteorology, potential source regions, PM formation mechanisms, and types of sources. Thus, this task will encompass an investigation and summary of boundary conditions for at least these three meteorological regimes.

Scope of Work

The scope of work consists of four elements.

1.   Literature Review

We will perform a brief literature review to more fully describe the background concentration concepts (i.e., reach consensus on the definition of background and boundary sites) and investigate tropospheric and California background concentrations. We will review and summarize previous boundary and background concentrations for central California and for clean Pacific air (such as data collected at Mauna Loa) to provide contrast and a point of reference for the present study. Summaries of $PM_{2.5}$ data collected in the San Francisco Bay Area and SJV will be most useful although ozone studies will also provide useful information on summer conditions (e.g., Blumenthal et al., 1997). Previous studies in the Sacramento and Shasta County areas will provide information about the Northern Border (e.g., Main et al., 1996). VOC concentrations from long-term trends sites and the PAMS program have been documented by Main et al. (1999). $PM_{2.5}$ concentrations in the SJV have been reported by many investigators including Chow et al., (1996).

This task will be limited to new and updated literature. To the extent that new information is available, we will review and summarize previous boundary and background concentrations for central California and for clean Pacific air and summarize the results in a final memorandum. We will use our previous study results and the literature review results to develop ranges of concentrations that are representative of background and clean air boundary sites. These ranges will then be used to develop selection criteria to help in the selection of sites and time periods for further analysis.

2.   Assess data availability and select sites and time periods for study.

In this task element, we will select time periods, sites, and potential data sets for further investigation into boundary conditions. We will use the results of other tasks, summaries of episode concentrations and meteorology, and discussions with other investigators.

Boundary and background sites will vary with the type of meteorological/episode conditions. CRPAQS sites are summarized in the field plan and include a combination of full-scale anchor monitoring sites measuring both gaseous and aerosol species; supplemental satellite sites measuring aerosol species using portable monitors; and a backbone network of existing California Air Resources Board (ARB) and air pollution control district sites. Sites along the west coast, in the Sierra Nevada and in the southeast and Owens Valley were intended to best represent background concentrations and composition. Watson et al. (1998) list the following sites that are of potential use in this task:

- *Background* – D.L. Bliss State Park, Dome Land Wilderness, Point Arguello, Point Arena, Pinnacles National Monument, Point Reyes National Seashore, Sequoia National Park, South Lake Tahoe, Yosemite National Park Turtleback Dome, and Bodega Bay .

- *Rural intrabasin gradient* – Angiola, Cantil, Carrizo Plain, Coalinga, Crows Landing, Dublin, Edison, Edwards AFB, El Rio, Foothills, South Fresno, Helm, Jackson, Kettleman City, Kern, Piru, Pleasant Grove, Portola, Roseville, San Andreas, Sierra Nevada Foothills, Chowchilla, Victorville, Yuba City, and Yosemite Village.

- *Mountain pass sites for interbasin transport* – Altamont, Bouquet Canyon, Bethel Island, Sierra Nevada Foothills, Livermore, Pacheco Pass, Soledad Canyon, Tehachapi Pass, Tejon Pass, Vallejo.

Available measurements at these sites vary (e.g., see Watson et al., 1998). For all three site types listed, an understanding of winds and mixing height will be useful in assessing the data collected at the sites (i.e., Task 5, particularly Task 5.2). Mixing height information will be especially crucial in understanding concentrations at the interbasin transport sites.

Data types for which boundary conditions need to be characterized include $PM_{2.5}$ mass, VOCs, NO_x, SO_2, and $PM_{2.5}$ composition including black carbon, OC, EC, sulfate, nitrate, trace elements (including marine aerosol tracers), and ions. We need these data for the sites of interest as well as surface wind speed and direction data. It would be useful to have the site and season specific relationship between b_{sp} and $PM_{2.5}$ mass so that b_{sp} data (which were available at more sites than $PM_{2.5}$ data) may be used to aid in establishing boundary conditions.

We intend to focus our analyses on 1-hr and 24-hr average data. Prior to data analysis, we will review the documentation accompanying the data to best understand any existing quality issues including time periods with missing or invalid data. We assume that the desired measurements will be available from the CRPAQS data management system in common formats.

3.   Characterize the boundary conditions

Methodologies available for the analysis of boundary conditions include trajectory analysis, spatial plots of selected statistical metrics (such as average concentration during like days), and visual displays of data including box plots and time series, and investigation of summary statistics. To best use available resources and integrate this task element with other tasks, we have identified analysis products that we need from other tasks and the analyses we plan to perform in this element. The general approach to this task element will be to

- identify time periods and episodes of interest starting with the list of episodes produced by ARB;

- use meteorology and descriptive summaries of the data to identify potential boundary sites during these episodes;

- review work products from other researchers;

- obtain necessary data;

- apply other statistical methods (such as cluster analysis) to investigate the relationships among the potential sites;

- finalize selection of boundary sites and data collection periods; and

- summarize the characteristics of the PM and precursor boundary conditions for the three modeling episode types.

By using a wide range of analyses, we can look for consensus among the results to establish our confidence in identifying boundary sites and in characterizing the concentrations at those sites.

We will first review critical results and data displays from Tasks 2.2 and 2.3 (and others) to prepare a preliminary selection of time periods and potential data sets for further investigation into boundary conditions. We will use selection criteria developed as a result of the literature review to provide a setting for our review of the data and for our discussions of the data with other investigators.

Using results from other task elements as described previously, we will assess typical meteorology during the three regimes that lead to episodes of high PM in the SJV. Using these meteorological assessments, we will then select sites that appear likely as boundary sites (i.e., upwind of the valley and major source areas). The concentrations at these sites before, during, and after the episode will be assessed using time series plots, box plots, and other spatial depictions of the data; these plots should be available from Tasks 2.2 and 2.3. We will include a comparison of the concentrations at the potential boundary sites with concentrations in the rest of the domain.

Our concept of clean air is air that has been transported for numerous days without any fresh emission inputs, such as might be expected for air that is transported across the Pacific Ocean. Since it is not practical to prepare air parcel trajectories of all the ambient samples in the study, criteria could be applied to select samples. For example, Collins used < 20% of mean sample levels as a selection criterion to separate clean background samples from other ambient

samples at a site. We intend to inspect the concentration distributions at selected boundary sites to investigate the feasibility of using 20% of the mean as a cut-off. A higher or lower cut-off concentration may be needed to best fit the data. Different cut-off criteria may be needed for different meteorological conditions (and/or seasons) as well.

Background criteria need to be applied separately to different compound classes and to different episode types. We will use information collected during a brief review of the literature pertaining to tropospheric background concentrations in general and California "background" concentrations specifically to aid in setting the criteria. Potential screening criteria include not only PM mass or component levels, but also ozone concentrations (summer), NO_x concentrations (all events), light scattering (all events), and selected ratios of pollutants.

We plan to augment descriptive displays of data from other tasks (such as Task 2.2) to further investigate relationships among species and sites. For example, we may prepare time series plots of selected pollutants and time periods using different groupings of sites than were previously prepared. One way to facilitate this would be to have access to the data files used to create the plots (e.g., Excel) so that simple changes could be made.

For those data summaries that are not available through the data management system or other tasks, but that are critical to our understanding of the data, we will compute summary statistics (distribution, minimum, maximum, median, average, confidence interval, coefficient of variation) of PM mass, PM composition, and PM precursors by site, time of day, day of week, episode, month, and season to investigate data at the boundaries. SYSTAT statistical software facilitates this (with batch processing). We will also use SYSTAT to prepare scatter plots, scatter plot matrices, and correlation tables of selected pollutants at individual sites or among sites to obtain an understanding of the relationships among potential boundary sites. These data summaries will assist us in understanding the spatial and temporal variation in the PM and precursor concentrations. This overall understanding of the data is critical to selecting and understanding the boundary sites.

For the summer and fall/winter transport conditions, trajectories would be useful to investigate the origin of air parcels during sampling – for example, did the air parcel travel over source areas? We propose to perform backward trajectories using HYSPLIT or wind modeling proposed to be performed by STI in Tasks 5.2 (CALMET) or use results from the ARB for selected sites and episodes. We will work with in-house meteorologists and the results of other analyses to select the appropriate heights for the trajectories (e.g., considering mixing heights, terrain, etc.). These heights may vary from episode to episode especially between the summer and fall/winter transport regimes. Trajectories at two different heights and from at least two times during the 24-hr sampling period (in the case of 24-hr average samples) can provide useful information about estimates of the path of the air parcels. Trajectories are not useful for stagnation periods except possibly for the days leading up to the episodes.

We will prepare selected descriptive displays of data to augment those received from other tasks (such as Task 2.2) to further investigate relationships among species and sites including

- time series plots of selected pollutants and time periods using different groupings of sites than were previously prepared;

- box plots of concentrations or ratios by site, time of day, day of week, and month as needed using SYSTAT statistical software to augment products from other tasks;

- scatter plots, scatter plot matrices, and correlation tables of selected pollutants at individual sites or among sites to obtain an understanding of the relationships among potential boundary sites;

- summary statistics (distribution, minimum, maximum, median, average, confidence interval, coefficient of variation) of PM mass, PM composition, and PM precursors by site, time of day, day of week, episode, month, and season to investigate data (for those data summaries not available through the data management system);

- spatial maps of selected episodes or data subsets as needed to augment other task products.

All these analyses will be used to establish selection criteria for boundary conditions. We will then prepare summary statistics of concentrations at the boundary for selected meteorological conditions.

4.   Documentation

We will summarize the results of task elements 1 through 3 in a memorandum and draft paper for publication. A brief outline of these documents follows:

Abstract
Implications Statement (if prepared for AWMA)
Introduction and Task Objectives
Definitions, Selection Criteria, and Episode Types
Available Data
Overview of Technical Approach and Analysis Techniques
Summer Transport Boundary Conditions
Fall/Winter Transport Boundary Conditions
Winter Stagnation Boundary Conditions
Conclusions
References

Time Line

Task 1 can commence immediately; however, other work depends on the availability of results from several other tasks. We anticipate that STI's boundary analyses will not begin until spring 2003.

Schedule of Deliverables

Table 1. Estimated schedule of deliverables.

Deliverable	Deliverable Date
Submit Draft Work Plan	December 2002
Submit Revised Work Plan	January 2003
Perform literature review	January 2003
Receive preliminary products from Tasks 2.2, 2.3, 3.3, and 5.2	March 2003
Obtain data	April 2003
Receive preliminary products from Task 4.1, 4.4	April 2003
Prepare data summaries to augment products of other tasks	June 2003
Perform remaining analyses	July 2003
Submit draft final memorandum	August 2003
Attend Mid-project Meeting	Summer 2003
Receive comments on draft final memorandum	September 2003
Submit Final Memorandum	October 2003
Present findings at annual conference	Fall 2003
Submit peer-reviewed paper	December 2003

Description of Deliverables

- A summary of literature-derived background and boundary concentrations for PM and its precursors
- A draft technical report documenting our results
- A final memorandum incorporating reviewer's comments
- A presentation for a conference (e.g., 2003 AWMA Annual Conference)
- A paper to be submitted for publication based on the report

ARB Staff Assigned to This Task

The ARB Project Manager assigned to this Task is

Theresa Najita
Planning and Technical Support Division

Mailing Address:

California Air Resources Board
P.O. Box 2815
Sacramento, CA 95812
Ph.: (916) 322-7297
e-mail: tnajita@arb.ca.gov

STI Staff Assigned to This Task

The STI Project Manager is Lyle R. Chinkin. The STI Task Manager assigned to this task is Hilary R. Hafner.

Data Products to be Performed/Delivered by ARB

To investigate boundary conditions, there are many analyses, particularly descriptions and displays of the data, that need to be carried out for a thorough understanding of the data. Many of these analyses are outlined as part of other tasks in the overall CRPAQS analysis effort. To carry out Task 2.4 efficiently, both the budget and schedule will be dependent on these tasks. Specific needs for the boundary conditions analyses are summarized in the following tables:

Table 2.   Data needs for Task 2.4 (products from other analyses).

Source/Tasks	Products needed for boundary conditions
ARB/Task 2.2 (spatial, seasonal, daily, and diurnal variations in PM mass, components, and precursors)	− Depictions and descriptions of the concentration distribution of pollutants at each site (i.e., lognormal) as a function of season. Histograms are useful in this regard. − Spatial plots (e.g., contour maps) of $PM_{2.5}$ mass, $PM_{2.5}$ components, and PM precursor concentrations or ratios including selected days, episodes, and seasonal summaries. Pertinent examples of the three types of meteorological conditions (i.e., summer transport, fall/winter transport, and winter stagnation) will be key. − Summary plots of spatial and temporal variation in the data including time series plots of pollutant concentrations or ratios at all sites (some of these plots will be available as a part of the CRPAQS data management system). − Box-whisker plots of PM and precursor concentrations or ratios by site, time of day, day of week, episode type, and month.

Table 2.   Data needs for Task 2.4 (products from other analyses).

Source/Tasks	Products needed for boundary conditions
ARB/Task 2.3 (ratio of $PM_{2.5}$ to PM_{10} and its spatial, diurnal, and seasonal variation)	− Spatial plots of $PM_{2.5}/PM_{10}$ ratios including selected days, episodes, and seasonal summaries. Pertinent examples of the three types of meteorological conditions (i.e., summer transport, fall/winter transport, and winter stagnation) will be key. − Time series plots of $PM_{2.5}/PM_{10}$ ratios for all sites. − Box-whisker plots of the $PM_{2.5}/PM_{10}$ ratios by site, time of day, day of week, episode type, and month.
ARB	− Wind fields for selected episodes, trajectory analyses.

Table 3.   Data needs for Task 2.4 (products from other analyses).

Source/Tasks	Products needed for boundary conditions
T&B/Task 3.3 and STI/Task 5.2 (meteorological phenomena, meteorology at transport pathways)	− Important meteorological phenomena including description of stagnation conditions and their extent in the SJV. − Mixing height estimates at interbasin transport sites on days of interest. − Description of transport during episodes. − Differences among episode types with respect to transport.
DRI/Task 4.1 (source apportionment)	− List of samples with high proportions of non-anthropogenic PM. − Identification of background sites and regional background composition based on modeling.
DRI/Task 4.4 (zone of influence)	− Description of the zone of influence of PM emission sources as a function of chemical constituent and particle size. − Discussion of how the zone of influence changes with space and time.

We will discuss our needs with the principal investigators of the above tasks to avoid duplication of effort and to maximize the investigative potential of the budgets.

Software and Models To Be Used by STI

STI intends to use the following publicly available software on this project: Microsoft Access, Excel, and Word; SPSS SYSTAT; and source apportionment software UNMIX and PMF.

Models, Reports, or Other Data to be supplied to STI by ARB

Table 4. Data needs for Task 2.4 (sites, data types, and data intervals).

Sites	Data types	Data duration
• *Background* - D.L. Bliss State Park, Dome Land Wilderness, Point Arguello, Point Arena, Pinnacles National Monument, Point Reyes National Seashore, Sequoia National Park, South Lake Tahoe, Yosemite National Park Turtleback Dome, and Bodega Bay. • *Rural intrabasin gradient* - Angiola, Cantil, Carrizo Plain, Coalinga, Crows Landing, Dublin, Edison, Edwards AFB, El Rio, Foothills, South Fresno, Helm, Jackson, Kettleman City, Kern, Piru, Pleasant Grove, Portola, Roseville, San Andreas, Sierra Nevada Foothills, Chowchilla, Victorville, Yuba City, and Yosemite Village. • *Mountain pass sites for interbasin transport* – Altamont, Bouquet Canyon, Bethel Island, Sierra Nevada Foothills, Livermore, Pacheco Pass, Soledad Canyon, Tehachapi Pass, Tejon Pass, Vallejo.	• $PM_{2.5}$ mass, VOCs, NO_x, SO_2, and $PM_{2.5}$ composition including black carbon, OC, EC, sulfate, nitrate, trace elements (including marine aerosol tracers), and ions • Surface wind speed and direction data • For the interbasin transport sites, mixing height information	• 1-hr and 24-hr average data • Data are required for three types of meteorological conditions

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